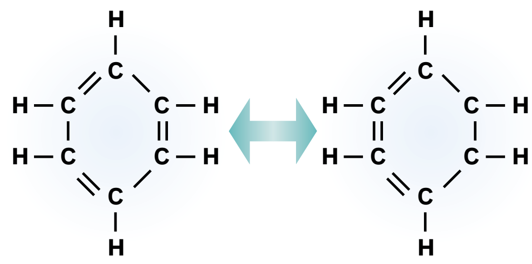

Figure 2.23: Aromatic hydrocarbons. *Benzene is soluble in water because of its "aromatic" structure.*

matic increase in solubility (to 82,000 mg/L). Adding a chloride atom to the benzene ring diminishes its aromatic character (chloride inhibits the dancing electrons), and thus the solubility of chlorobenzene (448 mg/L) is less than benzene.

Sorption

In the 1940s, a young pharmaceutical industry sought to develop medicines that could be transported in digestive fluids and blood (both of which are essentially aqueous solutions) and could also diffuse across cell membranes (which have, in part, a rather nonpolar character). The industry developed a parameter to quantify the polar versus nonpolar character of potential drugs, and they called that parameter the octanol-water partition coefficient. Basically they put water and octanol (an eight-carbon alcohol) into a vessel, added the organic compound of interest, and shook the combination up. After a period of rest, the water and octanol separate (neither is very soluble in the other), and the concentration of the organic compound can be measured in each phase. The *octanol-water partition coefficient*, or K_{ow}, is defined simply as:

$$K_{ow} = \text{concentration in octanol} / \text{concentration in water}$$

Table 2.7: Solubility of six-carbon compounds.

Compound	Solubility
Hexane	10 mg/L
Hexanol	5,900 mg/L
Cyclohexane	55 mg/L
Benzene	1,780 mg/L
Phenol	82,000 mg/L
Chlorobenzene	448 mg/L

The relation between water solubility and K_{ow} is shown in **Figure 2.24**. Generally we see that very insoluble compounds like DDT and PCBs have very high values of K_{ow}. Alternatively, organic acids and small organic solvents like TCE are relatively soluble and have low K_{ow} values.

The octanol-water partition coefficient has been determined for many compounds and can be useful in understanding the distribution of SOC between water and biota, and between water and sediments. Compounds with high K_{ow} tend to accumulate in fish tissue (**Figure 2.25**). The *sediment-water distribution coefficient*, often expressed as K_d, is defined in a sediment-water mixture at equilibrium as the ratio of the concentration in the sediment to the concentration in the water:

$$K_d = \text{concentration in sediment} / \text{concentration in water}$$

One might ask whether this coefficient is constant for a given SOC. Values of K_d for two polyaromatic hydrocarbons in various soils are shown in **Figure 2.26**. For pyrene (which consists of four benzene rings stuck together), the K_d ratios vary from about 10 to 1500. For phenanthrene (which consists of three benzene rings stuck together), K_d varies from about 10 to 300. Clearly K_d is not a constant value for either compound. But, K_d does appear to bear a relation to the fraction of organic carbon in the various sediments. What appears to be constant is not K_d itself, but the ratio of K_d to the fraction of organic carbon in the sediment. This ratio is referred to as K_{oc}: